Making Your Research Go Faster: Advanced HPCC CI-Days October 23, 2014

https://wiki.hpcc.msu.edu/x/5AJZAQ

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Agenda

- **Overview**
- Advanced System Description
- Powertools
- Doing more faster
  - Pleasantly Parallel, Shared Memory, Shared Network, Accelerators, Standard Libraries
- Tricks and tips

Assumptions

- You have logged in and used the HPCC or similar system
- You are familiar the the Linux command line
- You have some programming / scripting experience
- You are here to learn how to leverage HPCC resources better

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How this workshop works

- I think you work best from doing. So we will do a lot of hands on examples.
- When you get tired of listening to me talk, skip ahead to an exercise and give it a try.
- Exercises are denoted by the following icon in your notes:

Red and Green Flags

- Use the provided sticky notes to communicate without raised hands:
  - **NO Sticky** = I am working
  - **Green** = I am done and ready to move on
  - **Red** = I am stuck and need more time and/or I could use some help

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Submission Scripts

- Design Goals
  - One script does everything
  - Easy to read
  - Easily given to others
  - Easily moved to different directories

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What problems are we solving?

- Simulations
- Data Analysis
- Search

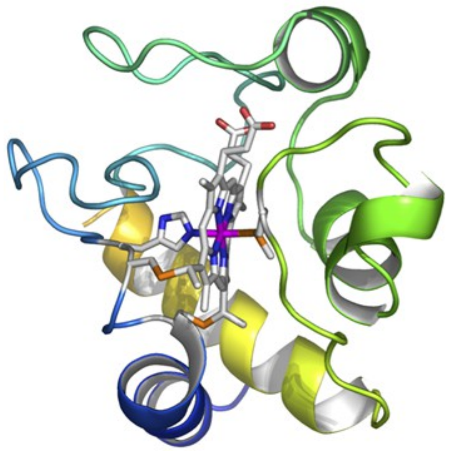
Image Provided by Dr. Warren F. Beck, MSU

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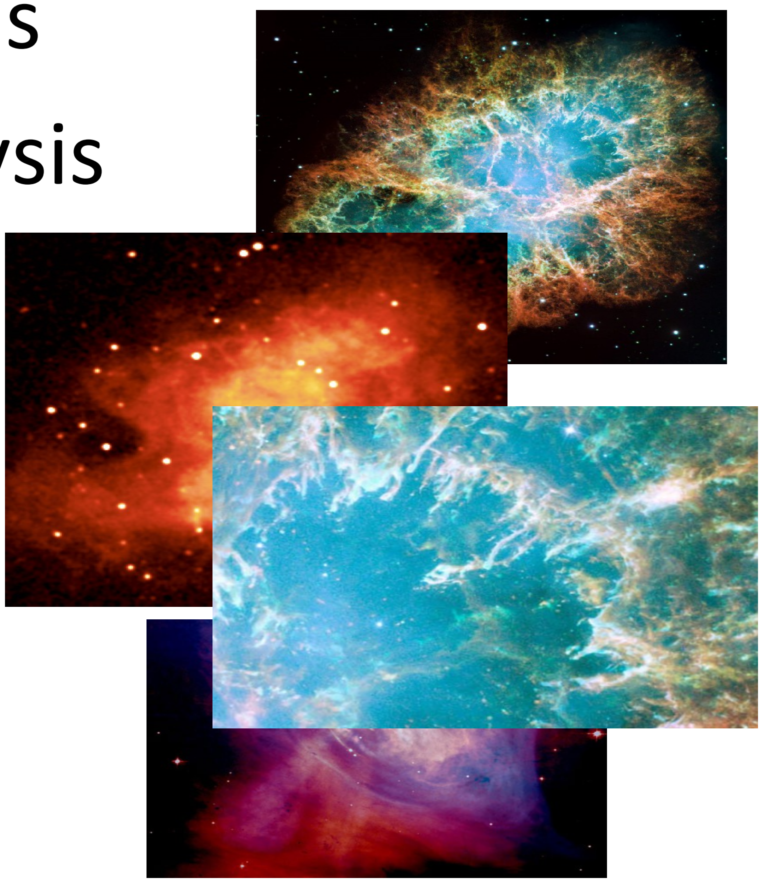
Images from, “Understanding the H_2 Emission from the Crab Nebula”, C.T. Richardson, J.A. Baldwin, G.J. Ferland, E.D. Loh, Charles A. Huehn, A.C. Fabian, P.Salomé

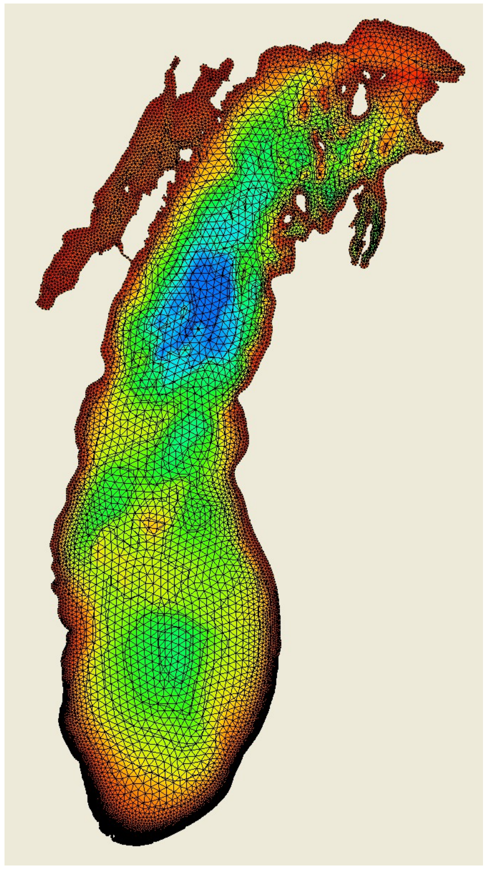
Image Provided by Dr. Mantha Phanikumar, MSU

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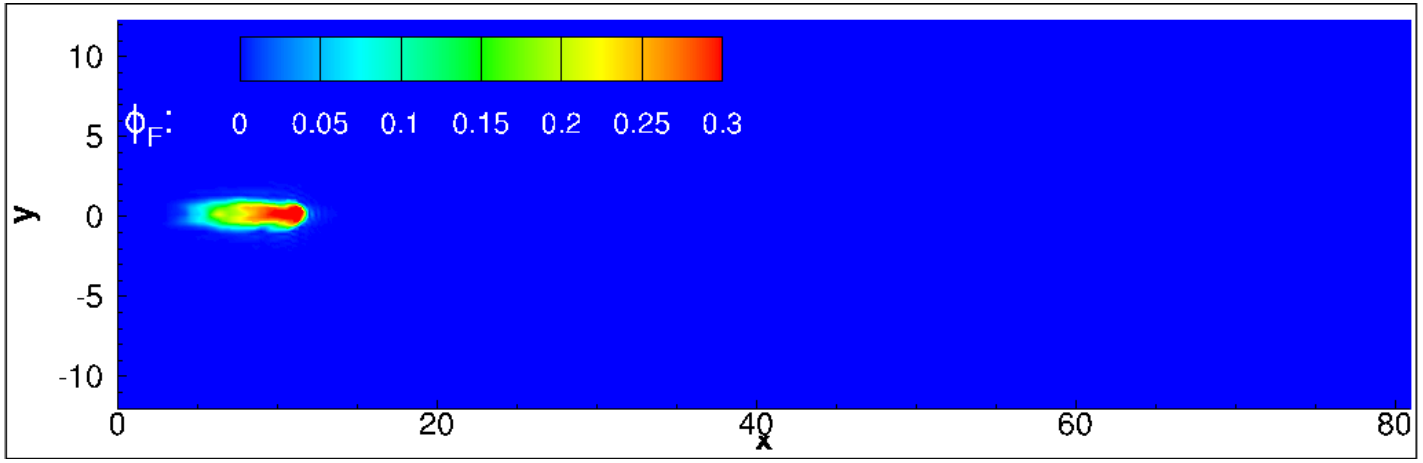
Simulations

- Typically System of PDE (Partial Differential equations)
  - Fluid dynamics
  - Finite element analysis
  - Molecular dynamics
  - Weather
  - Etc.
- Mathematically equivalent to inverse of a matrix



Premixed mixture of H2 -air auto igniting and flame propagation at supersonic flow
Provided by Dr Jabari and Mani (Abolfazl) Irannejad

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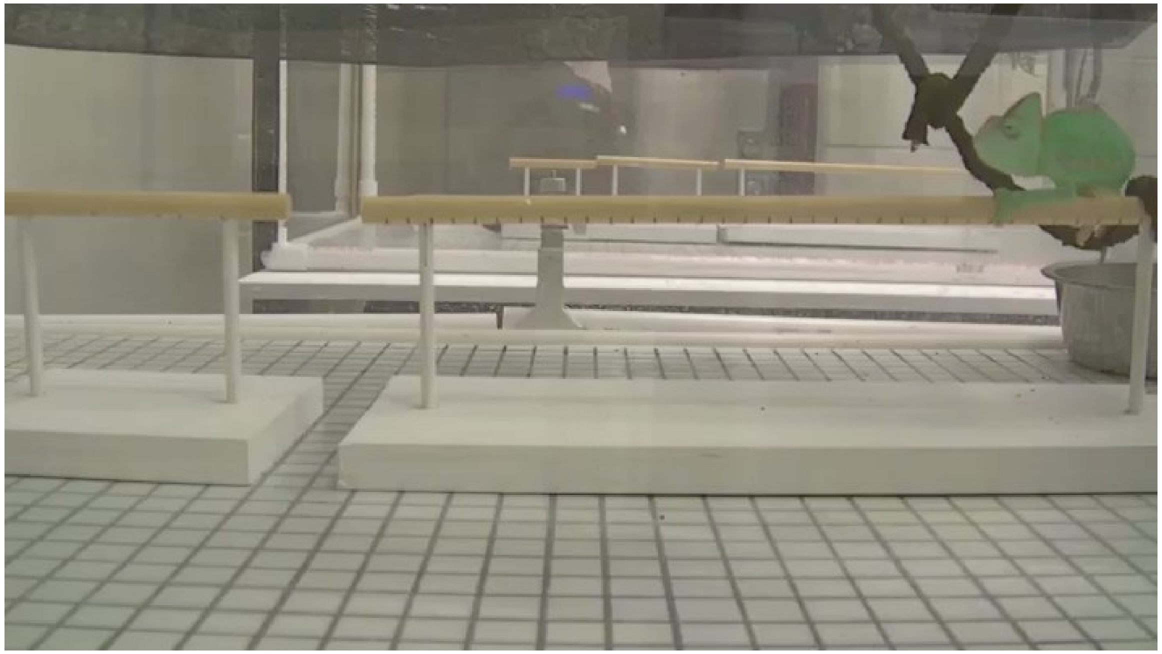
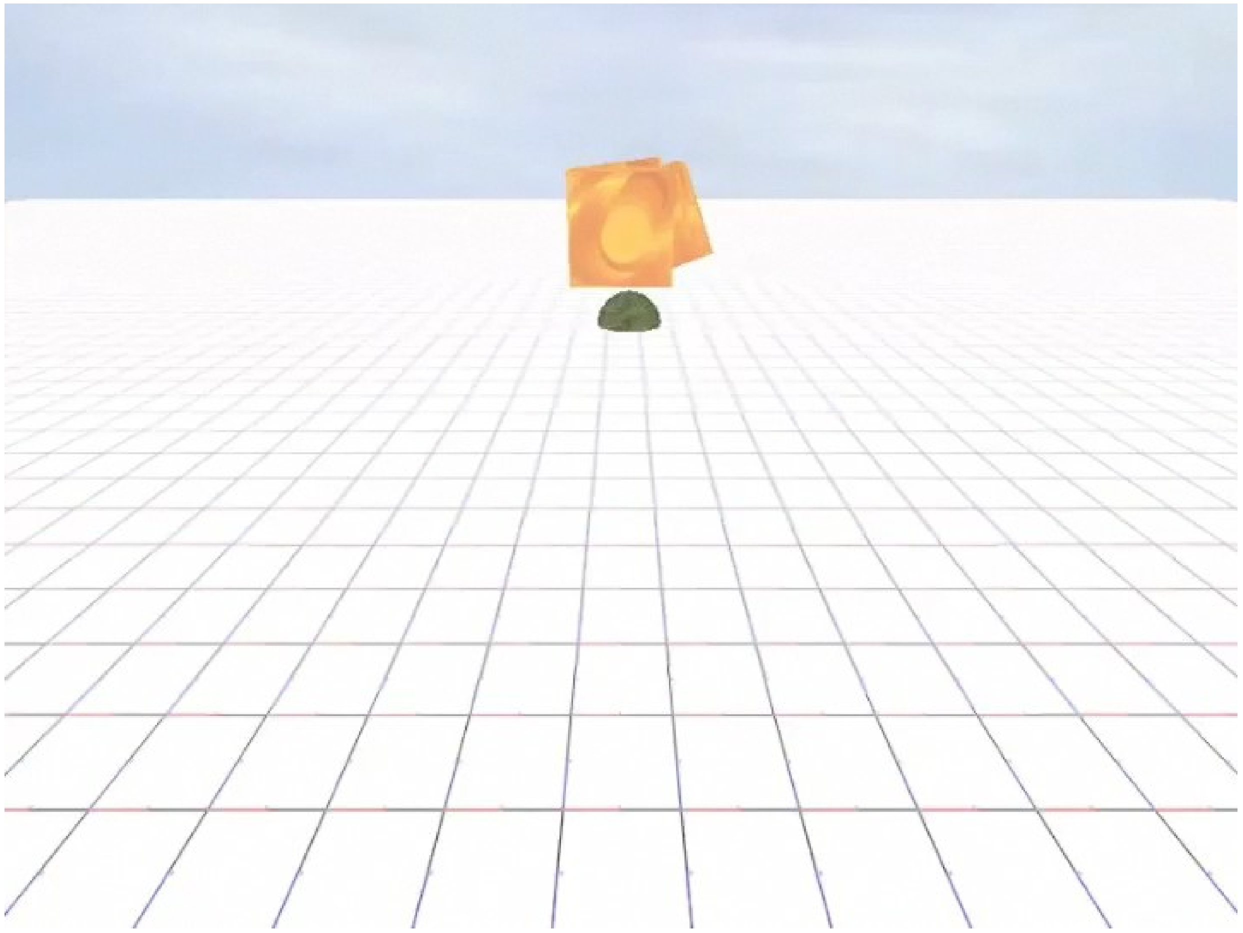
Data Analysis

- Computer vision tasks
- Some Bioinformatics
- Astrophysics
- Etc.


Video Provided by Dr. Fred Dyer

Search

- Genome sequencing
- Analytics
- Optimization
- Etc.


Evolution of an artificial organism that can move and forage for food, Dr. Nicolas Chaumont

HPC Systems

FREE*

- Large Memory Nodes (up to 6TB!`)
- GPU Accelerated cluster (K20, M1060)
- PHI Accelerated cluster (5110p)
- Over 600 nodes, 7000 computing cores
- Access to high throughput condor cluster
- 363TB high speed parallel scratch file space
- 50GB replicated file spaces
- Access to large open-source software stack and specialized bioinformatics VMs

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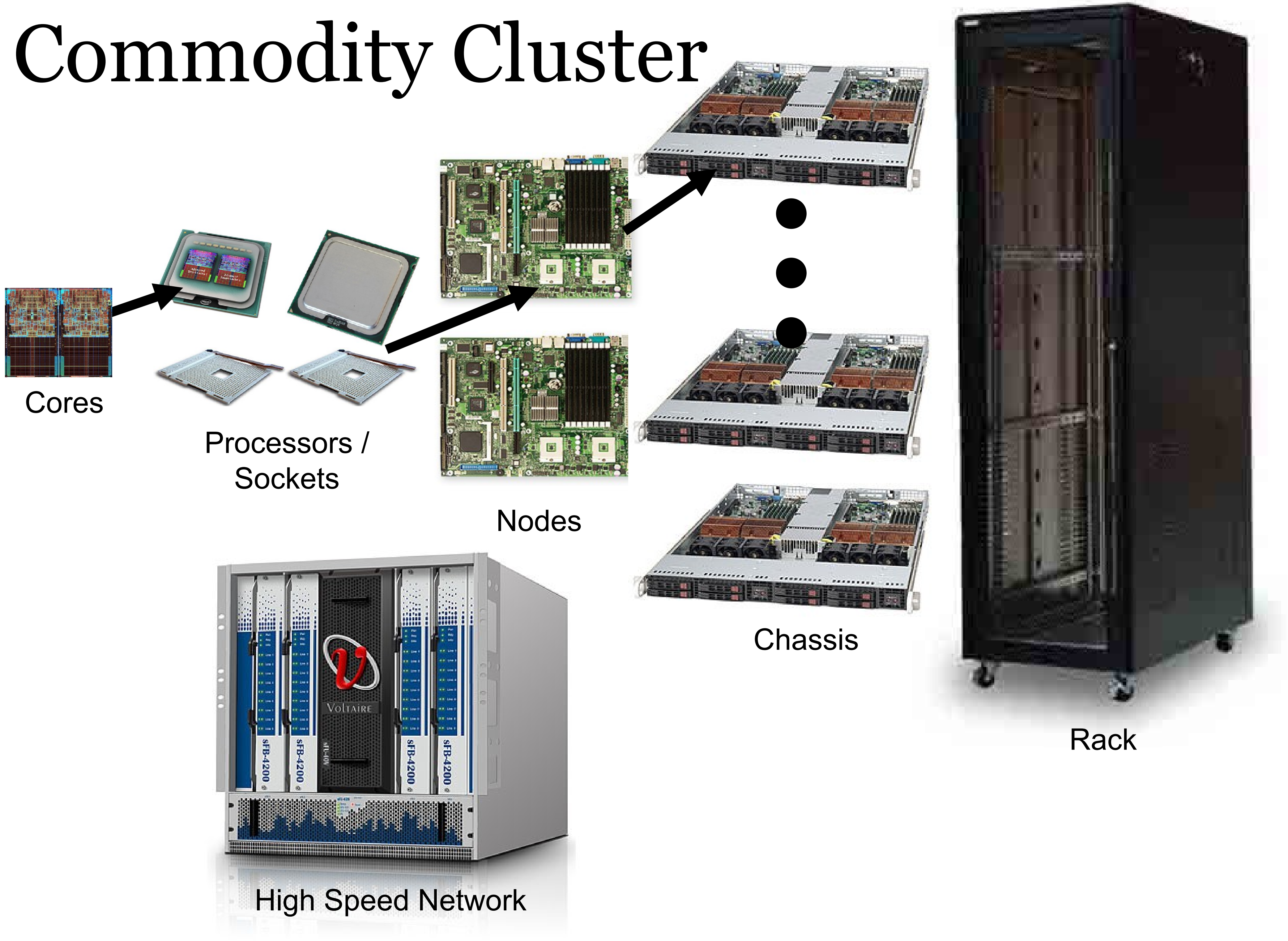
Free Access to software

- Compiled open-source software stack
  - Close to 2000 titles!
- Optimized Math/Communications libraries
- Some commercial software available
  - E.g. Ansys, MATLAB (+many toolboxes), Stata, Gauss, SAS

Full list: http://wiki.hpcc.msu.edu

General Purpose Clusters

Commodity Cluster



Buy-In Opportunities

- We will maintain your computers for you
- Researchers get exclusive use of their nodes within 4 hours of submitting a job
- Buy-in jobs will automatically overflow into the general resources.

Current Buy-In options (2014)

- 20 cores, 64 Gb, $3,806*
- 20 cores, 256 Gb, $5339*
- 20 cores, 128 Gb, 2 Nvidia K20, $7899*
- 20 cores, 128 Gb, 2 Intel 5115P, $9043*
- 48 cores, 1 Tb, $29,979
- 48 cores, 1.5 Tb, $34,989
- 48 cores, 3 Tb, $60,995
- 96 cores, 6 Tb, $142,772
- Replicated storage: $175/TB per year

* Some grant/funding agencies require a chassis for an additional $1216 (8 slots).

Large Shared Memory Systems (Fat Nodes)

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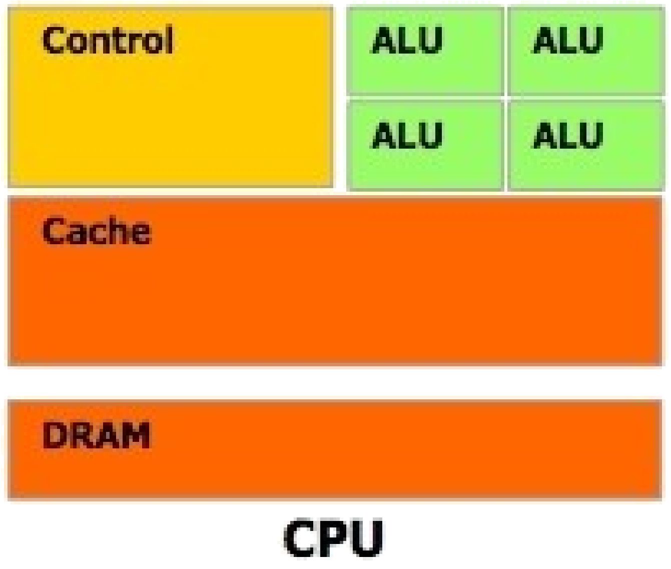
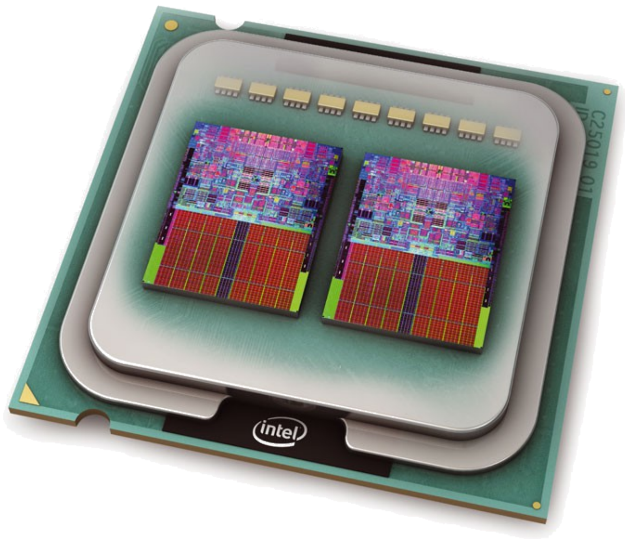
Shared Memory Communication

- Fast!
- Cores on a system share the same memory
- OpenMP
- Fat nodes
  - 96 cores
  - 6TB of memory





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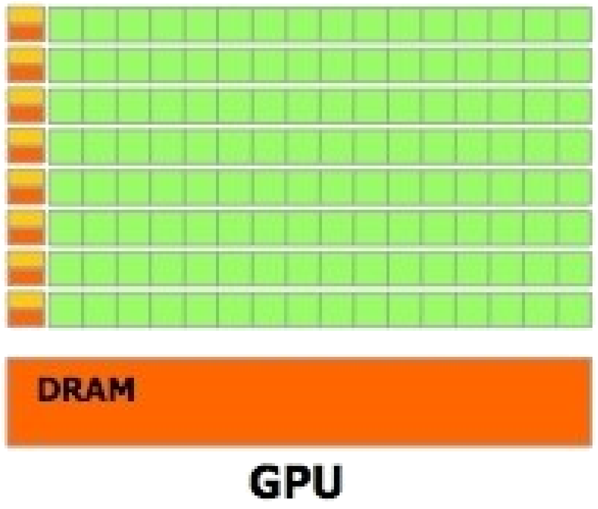
Accelerated Systems

GPU

- Cards used to render graphics on a computer
- Hundreds of cores
- Not very smart cores
- But, if you can make your research look like graphics rendering you may be able to run really fast!



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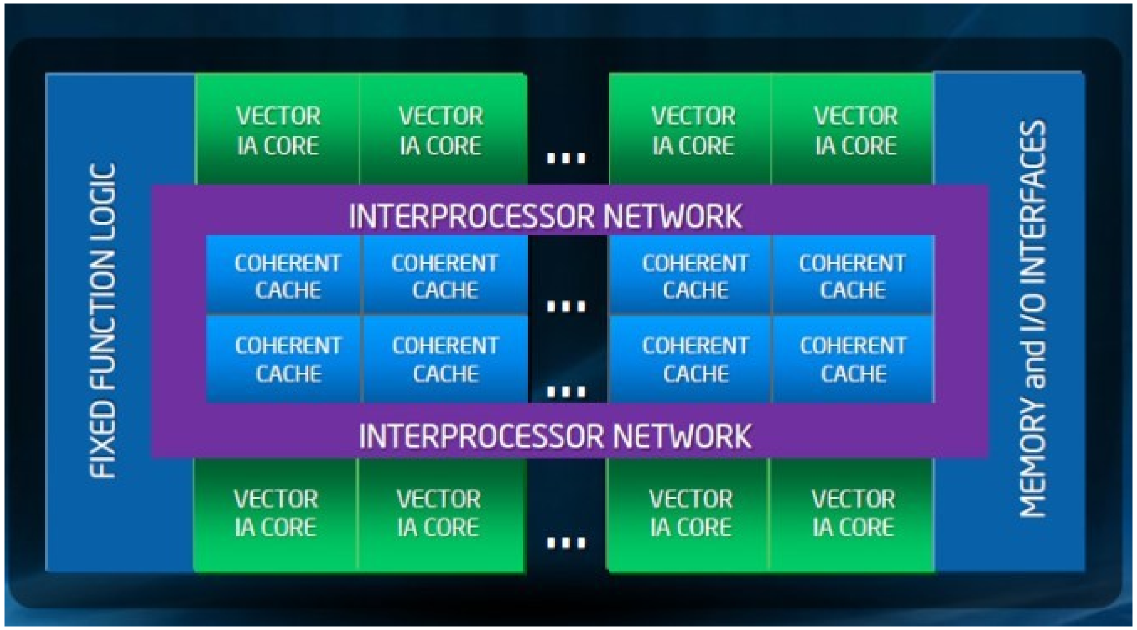
Intel Xeon Phi

- Cross between CPU and GPU
- About 61 Pentium III cores
  - Less cores/slower than GPU
  - Easier to use than GP



High Throughput HTCondor Cluster

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MSU HTCondor Cluster

- Runs like a screen saver and Scavenges CPU cycles:
  - Approximately 400+ nodes
  - Approximately 7000 cores
  - Windows 7

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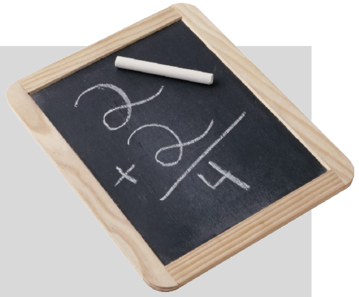
- Doing more faster
  - Pleasantly Parallel, Shared Memory Parallelization, Shared Network, Accelerators, Standard Libraries
- Tricks and tips

What are Powertools

- Powertools are scripts and programs to make interfacing with the HPCC simpler
- The tools are written mostly by HPCC staff and users.
- Think of most of these as “Beta” software.

How to Access Powertools



- When you are logged on to gateway or the developer nodes, load the powertools module file:

```
>module load powertools
```

- To list the currently available tools type “powertools” after loading the powertools module

```
>powertools
```

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Common Powertools

- Any developer node shortcut

```
> dev
```

- Developer node shortcuts

  (**intel07**, **gfx08**, **intel09**, **gfx10**, **gfx11, intel14**)

- Two commands in one:
  - Automatically ssh directly to the developer node
  - Then automatically cd to the current directory from the previous node

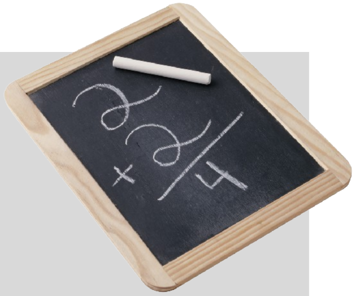
More Common Powertools

- **powertools** – list powertools and common commands not standard on linux systems
- **sj** – show jobs in the queue for the current user
- **starttime** – show estimated start times for a job
- **mailme** – E-mail yourself a file
- **clusterstate** – show a summary of the current state of the nodes in the cluster

Even More Powertools

- **getexample** – provides a copy of examples for various tasks written by iCER staff
- **quota** – list your home directory disk usage
- **priority_status** – Shows the status of an individuals buy-in nodes.
- **poweruser** – Set up your account to load powertools by default

How to turn on powertools as default?



- Edit your .bashrc

```
> nano ~/.bashrc
```

- add the following line:

```
module load powertools
```

Note: You can also just use the “**poweruser**” powertool

- Note: this is required if you want to use the developer node shortcuts and hop between different nodes

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- **Doing more faster**
  - **Pleasantly Parallel, Shared Memory Parallelization, Shared Network, Accelerators, Standard Libraries**
- Tricks and tips

What is the Bottleneck

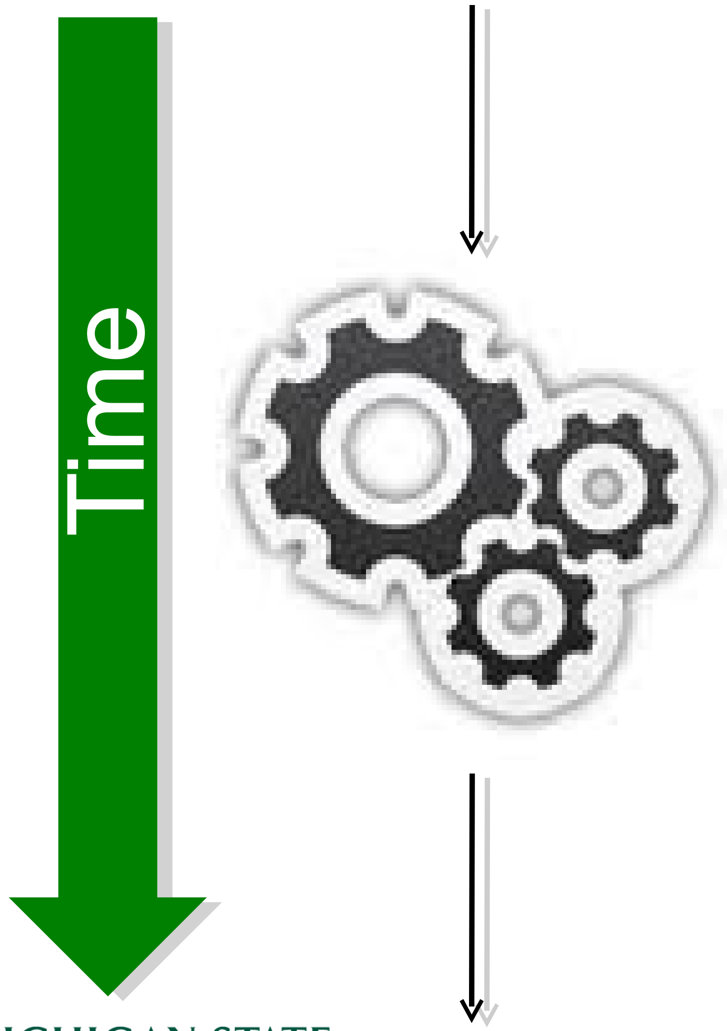
- Not enough Memory
  - Solution: use a bigger node (6tb 96 cores)
- Slow File I/O
  - Solution: use scratch
  - Solution: use a ram disk
- Too many calculations
  - Solution: run your code in parallel

Steps to parallel code

Note: Every application is different

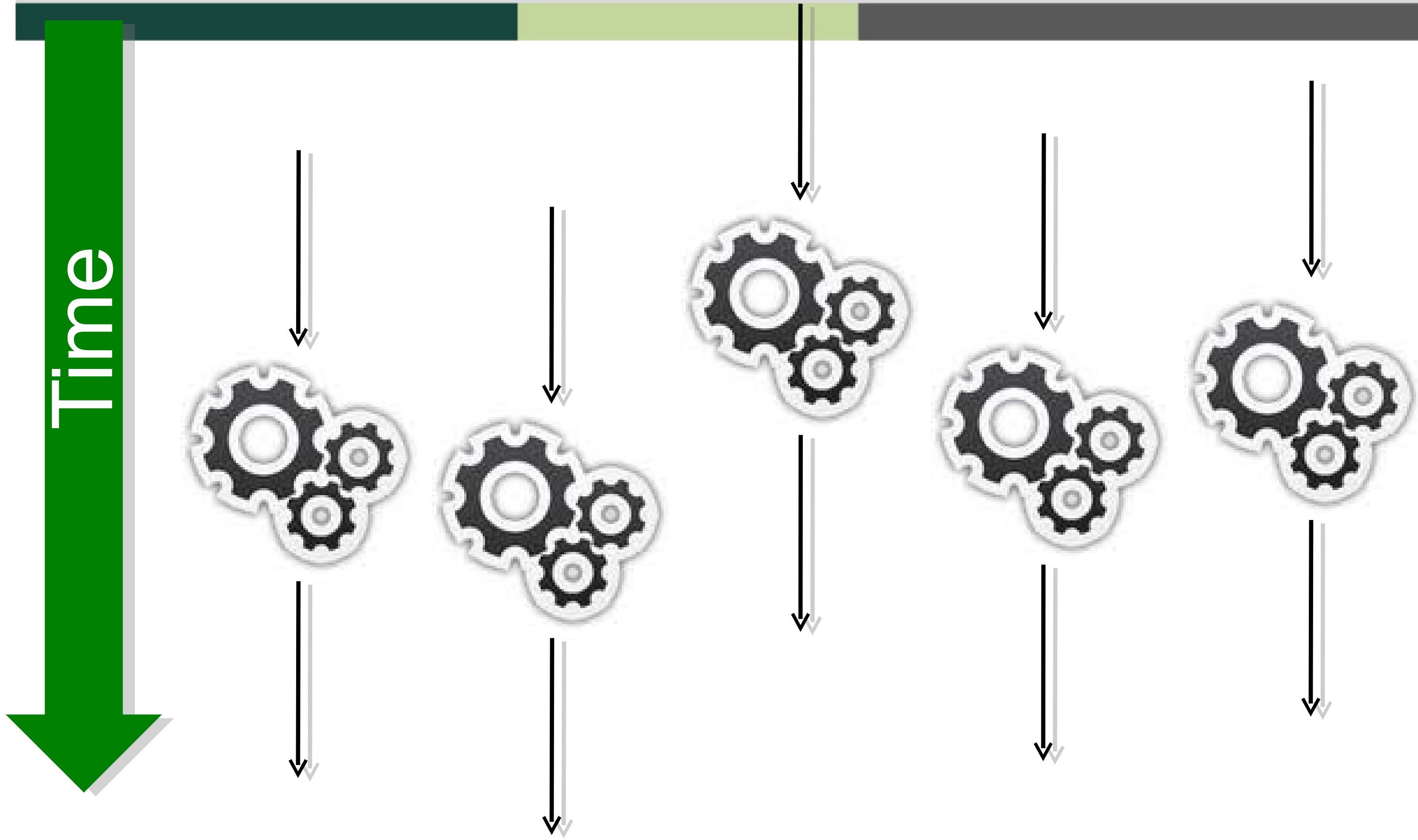
1. Analyze your code
   - Profilers (gprof, vtune, map, perfreport, tau)
   - Debuggers / memory trackers (gdb, ddt, totalview)
1. Optimize calculations
   - Trade memory for time (i.e., never do the same calculation twice)
1. Find ways to parallelize
   - Look for loops
   - Find iterations independent from each other
   - Determine how much information needs to be transferred

Single Thread Jobs

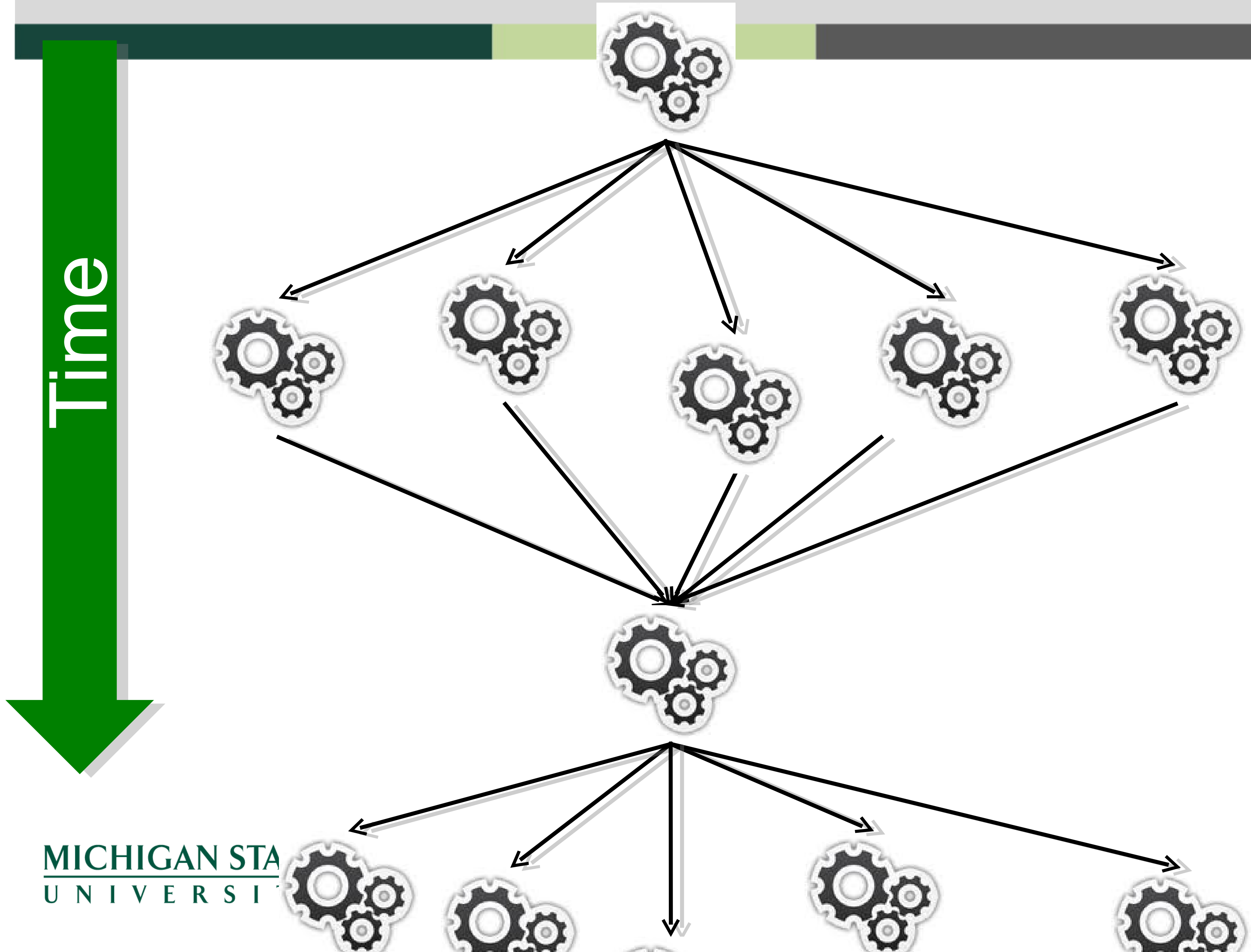


One CPU can only run one thing at a time. (sort of)

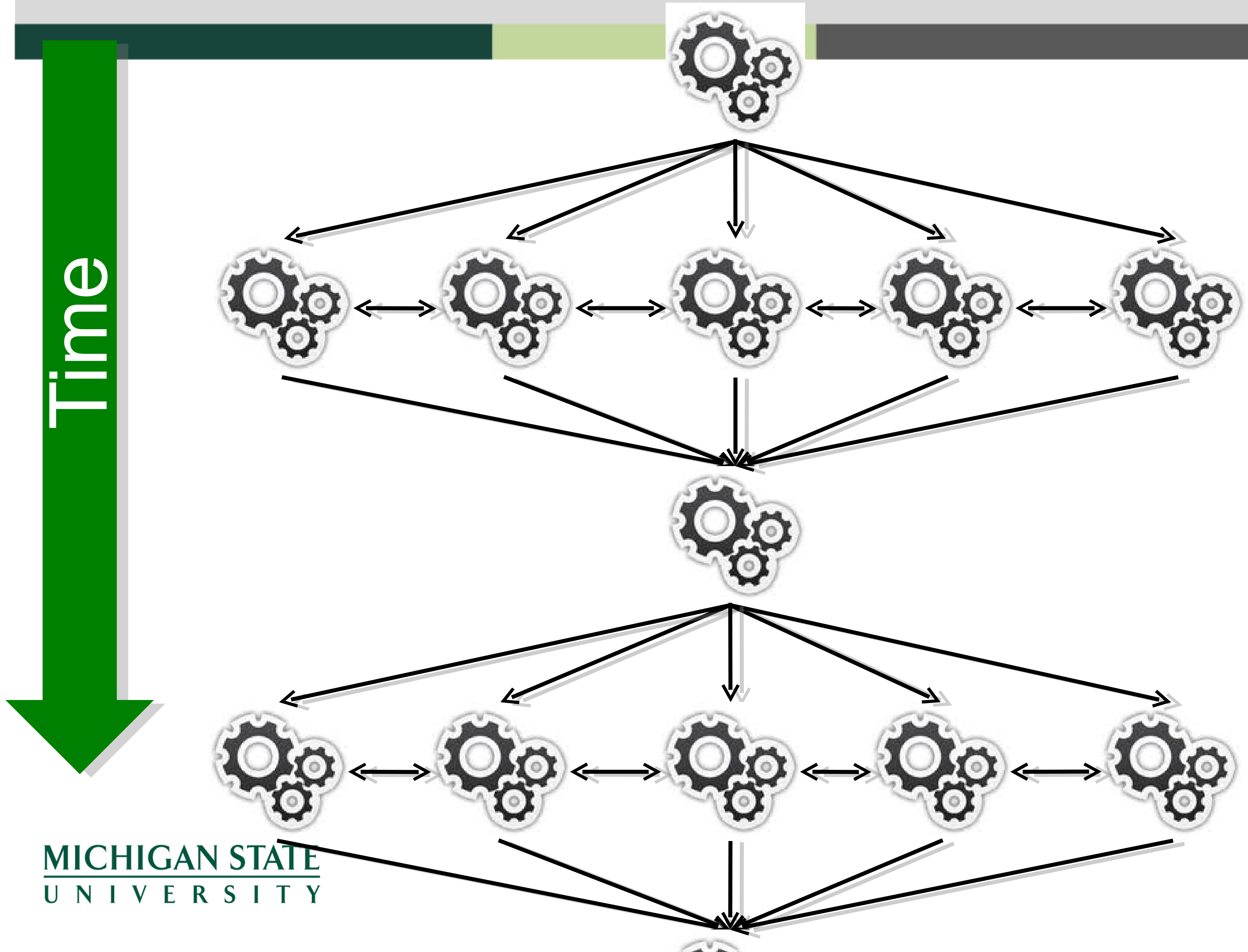
Pleasantly Parallel



Loosely Coupled



Tightly Coupled



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Communication

- Shared Memory
- Shared Network
- Distributed Network
- Dedicated Accelerators
- Hybrid Systems

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Pleasantly Parallel

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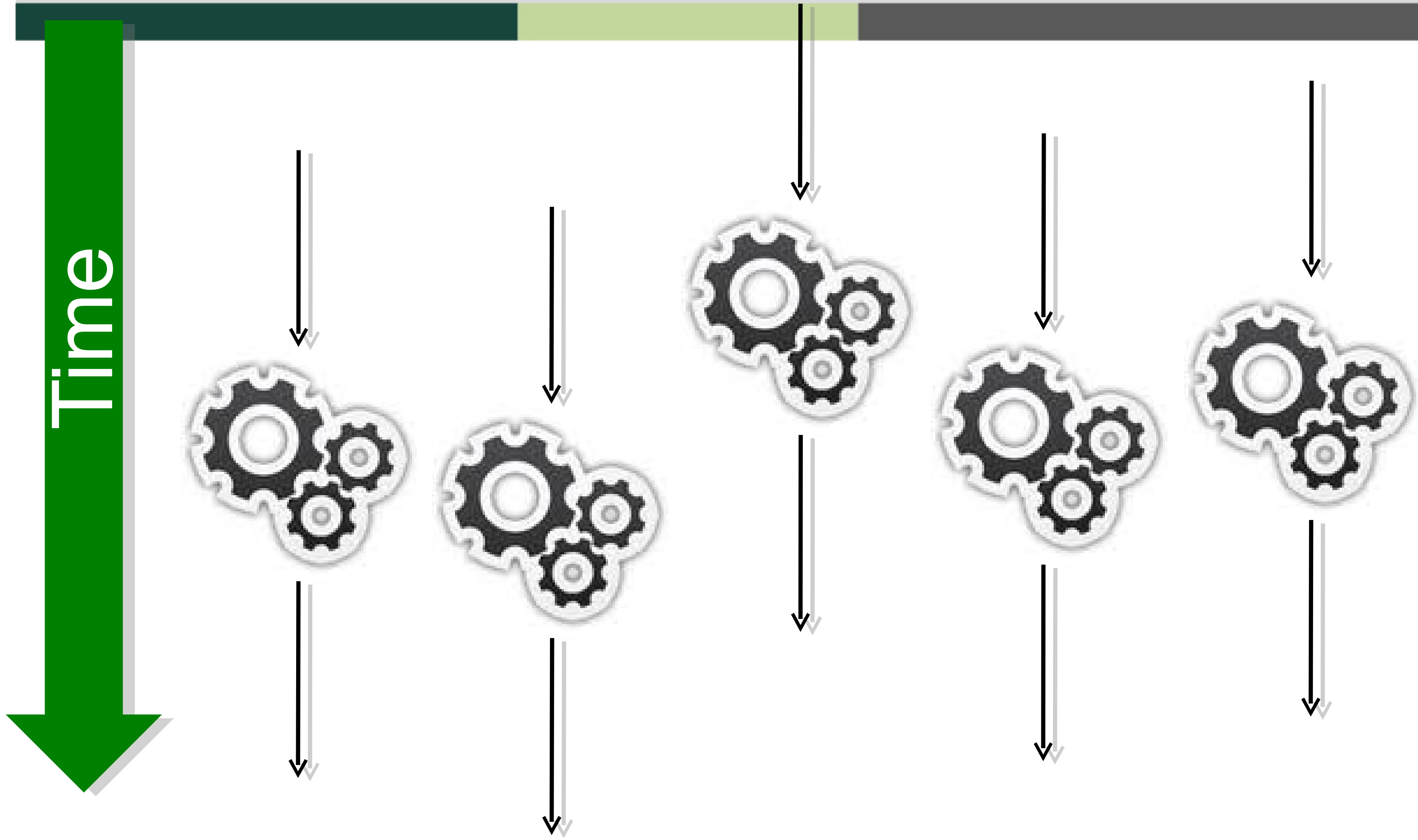
Pleasantly Parallel



How fast can we go?

- T - How long does each operation take?
- N - How many operations do you need to run?
- CPUs – Number of Cores job will run on.

- Single CPU time estimate:
  - TxN
- Best possible Pleasantly parallel time:
  - (TxN)*overhead/CPUs

Who are you? -- Biometrics

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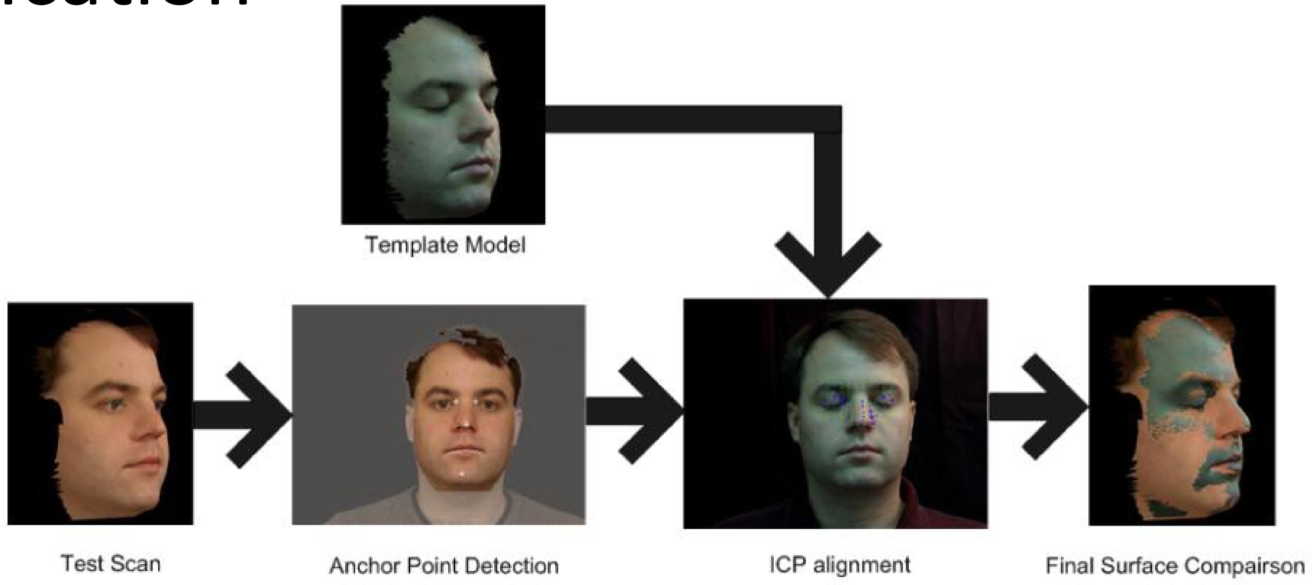
Pairwise-All Problem

- Database of faces
- Compare everything to everything else
- Calculate a Matching score to use for identification



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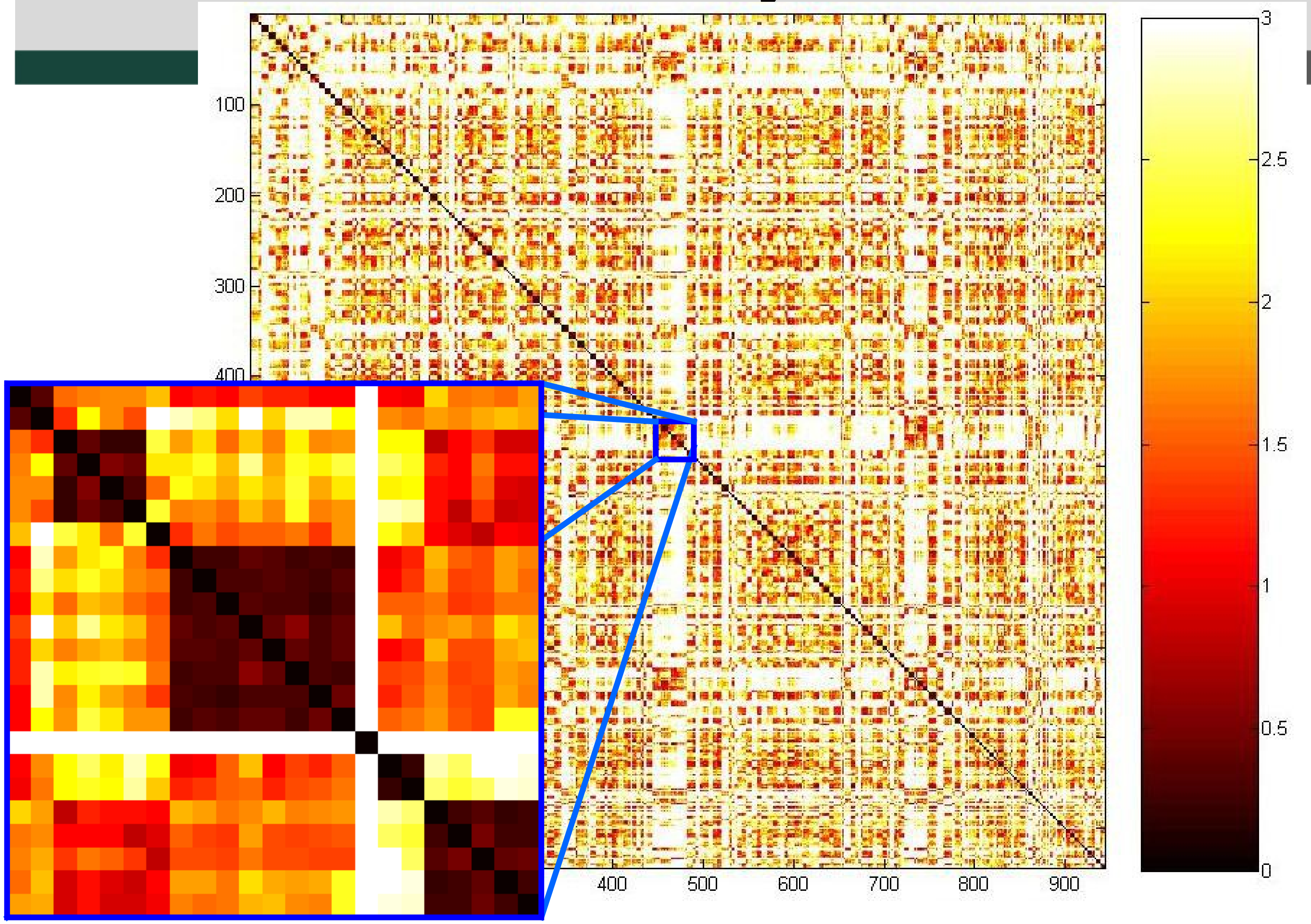
943 x 943 Similarity Matrix



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Estimated Calculation Times

- Preprocessing
  - 943 * 12 (seconds) ⁀ 189 Minutes
- Matching
  - 943 * 943 * 5 (seconds) ⁀ 103 Days
- Scans matched to themselves always result in 0 mm
  - (943 * 943 – 943) * 5 (seconds) ⁀ 103 Days
- The Proposed Alignment Algorithm is symmetric.
  - (943 * 943 – 943)/2 * 5 (seconds) ⁀ 51.5 Days
- We also load models once per row instead of every time
  - (943*943-943)/2 * 3 (seconds) + 943 * 2 (seconds) ⁀ 31 Days

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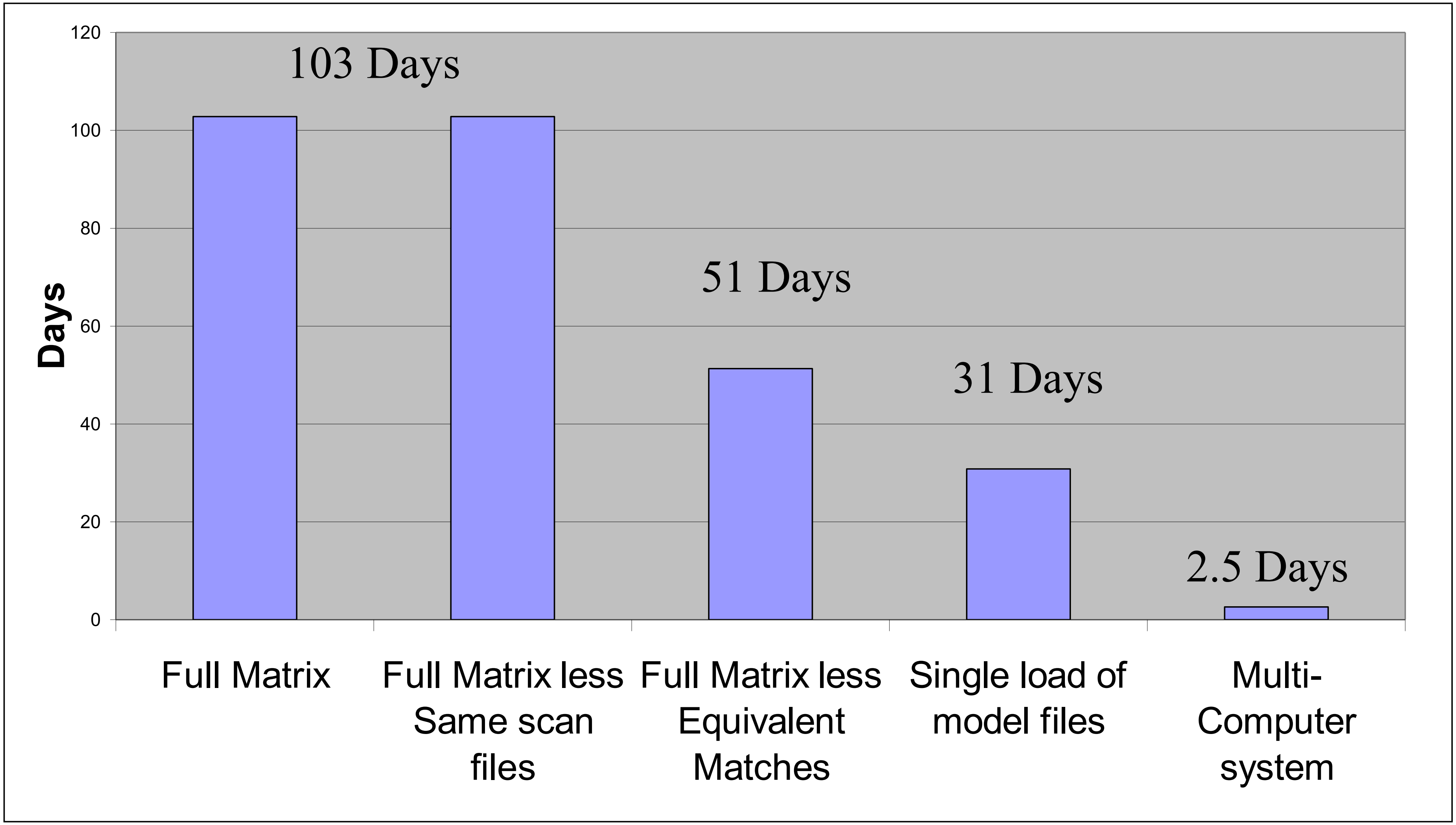
Calculation Time for Full Similarity Matrix



How do we go even bigger?

- 5000 scans.
  - 1.5 years on a single processor computer
  - 13 days on our ad-hoc cluster.
  - 1.5 days a commodity cluster at MSU

Steps to Pleasantly Parallel

- Figure out command line
- Estimate single job time:
  – Should be > 5 minutes
  – Should be < 1 week
  – Best if < 4 hours
- Make a submissions script
- Submit Job

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Pleasantly Parallel Example

- Folder full of input files:

1.in	5.in	9.in	13.in	17.in
2.in	6.in	10.in	14.in	18.in
3.in	7.in	11.in	15.in	19.in
4.in	8.in	12.in	16.in	

- Want folder full of output files:

1.out	5.out	9.out	13.out	17.out
2.out	6.out	10.out	14.out	18.out
3.out	7.out	11.out	15.out	19.out
4.out	8.out	12.out	16.out	

- Command Syntax:

```
./myprogram inputfile > outputfile
```

PBS Job Arrays

- One submission script copied many times
- Uses the PBS –t option
  - Ranges: 1-10
  - Lists: 2,4,100,3
  - Combination: 1-10,20,50,100
- Distinguish between jobs by using the PBS_ARRAYID environment variable

Simple Job Array

```
#!/bin/bash -login
#PBS -l walltime=00:05:00,mem=2gb
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-19

cd ${PBS_O_WORKDIR}

mkdir ${PBS_ARRAYID}
Cd ${PBS_ARRAYID}


../myprogram ../${PBS_ARRAYID}.in > ${PBS_ARRAYID}.out

qstat -f ${PBS_JOBID}
```

Example: Job Arrays

- Get the bleder_farm example:

```
> getexample
> getexample blender_farm
> cd ./blender_farm
```

- Look at the qusb file, using “less” command

```
> less blender_farm.qsub
```

- Submit the job

```
> qsub blender_farm.qsub
```

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HPCC Job array limitations

- Can not have more than 520 cores running at once
- Can not submit more than 1000 jobs at once
- Each job can not run longer than one week

- Lots of ways to work around these limitations

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Job array numbers

- All numbers in a job array have the same base number
  - 7478210
- Each PBS_ARRAYID is show in square brackets
  - 7478210[1]
  - 7478210[2]
- Delete all jobs using one command
  - qdel 7478210[]

Unrolling Loops

- Your program has independent loops
  - Each iteration of the loop does not depend on the other iterations
  - Loop can be executed in any order
  - 5 Minutes < Iteration Time < 1 week
  - Output of each iteration must be easy to save and recombine for next step of workflow

- Rewrite your program to accept an iteration number as an input
  - ./myprogram IterationNumber
- Rewrite your program to save output and use an additional program for post processing

Simple Unrolled Loop

```
#!/bin/bash -login
#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100

cd ${PBS_O_WORKID}

./myprogram ${PBS_ARRAYID}

qstat -f ${PBS_JOBID}
```

Task Queue

- A list of tasks (also called treatments, inputs, …) that distinguish what needs to be done.
- Each pleasantly parallel process (worker) checks the list and picks work not yet completed.
- The trick is to not have two workers do the same task.

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List of Commands

- Commands.txt

```
./myprogram -a 100 -z 3023
./myprogram dosomething different
./myprogram
./myprogram -s 100
./myprogram -s 200
./myprogram -s 300
./myprogram -w 400
./myotherporgram
./mythirdprogram
```

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List of Commands

```
#!/bin/bash -login
#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100

cd ${PBS_O_WORKID}

cmd=`tail -n ${PBS_ARRAYID} commands.txt | head -n 1`
echo ${cmd}
${cmd}

qstat -f ${PBS_JOBID}
```

Files as Semaphores (FAS)

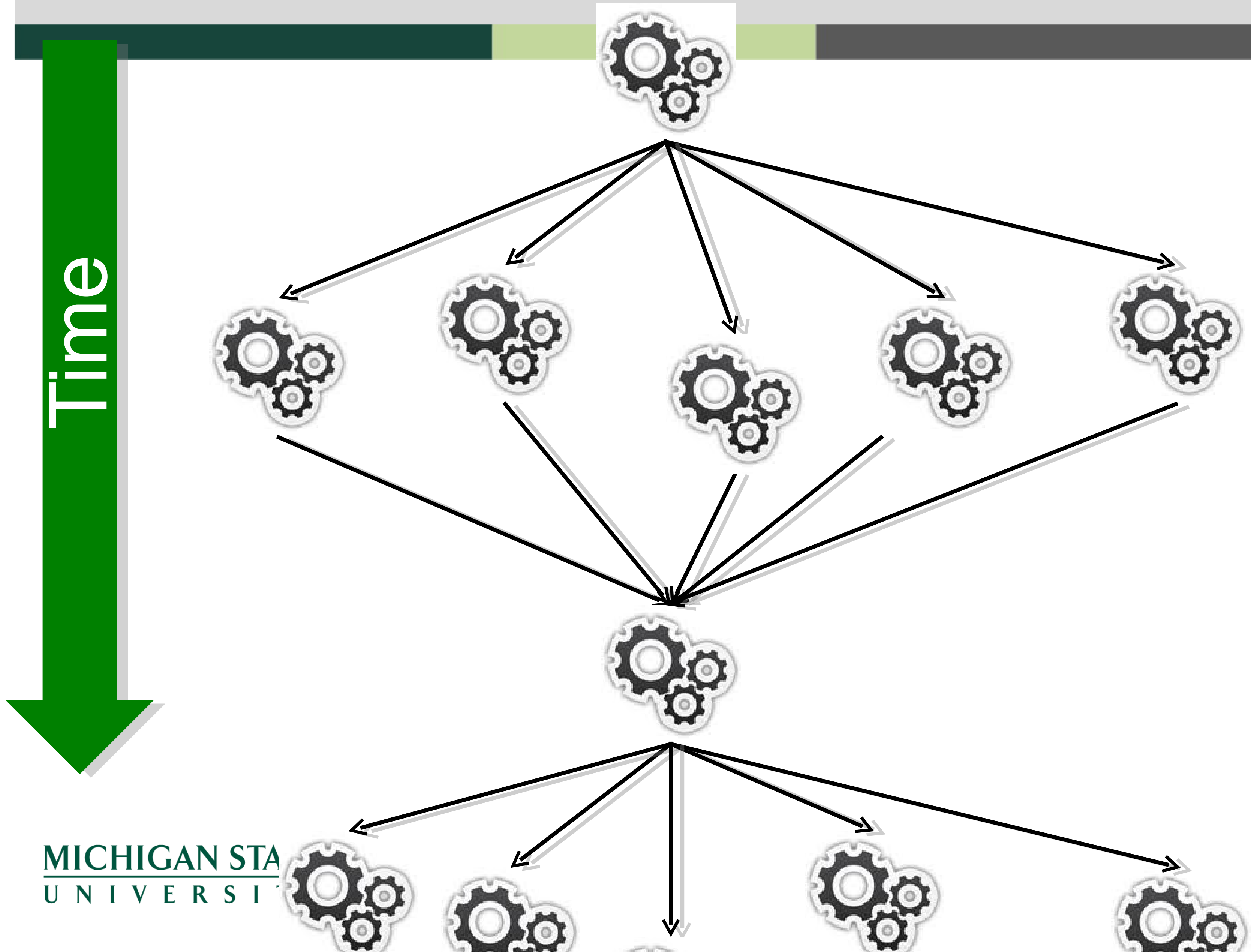
- Use a list of input files as your task list
- Use a list of output files (or flag files) as your in-progress/complete list
- Rely on the file system to ensure that no two jobs are selected at the same time (not a great assumption but it works)

Simple FAS

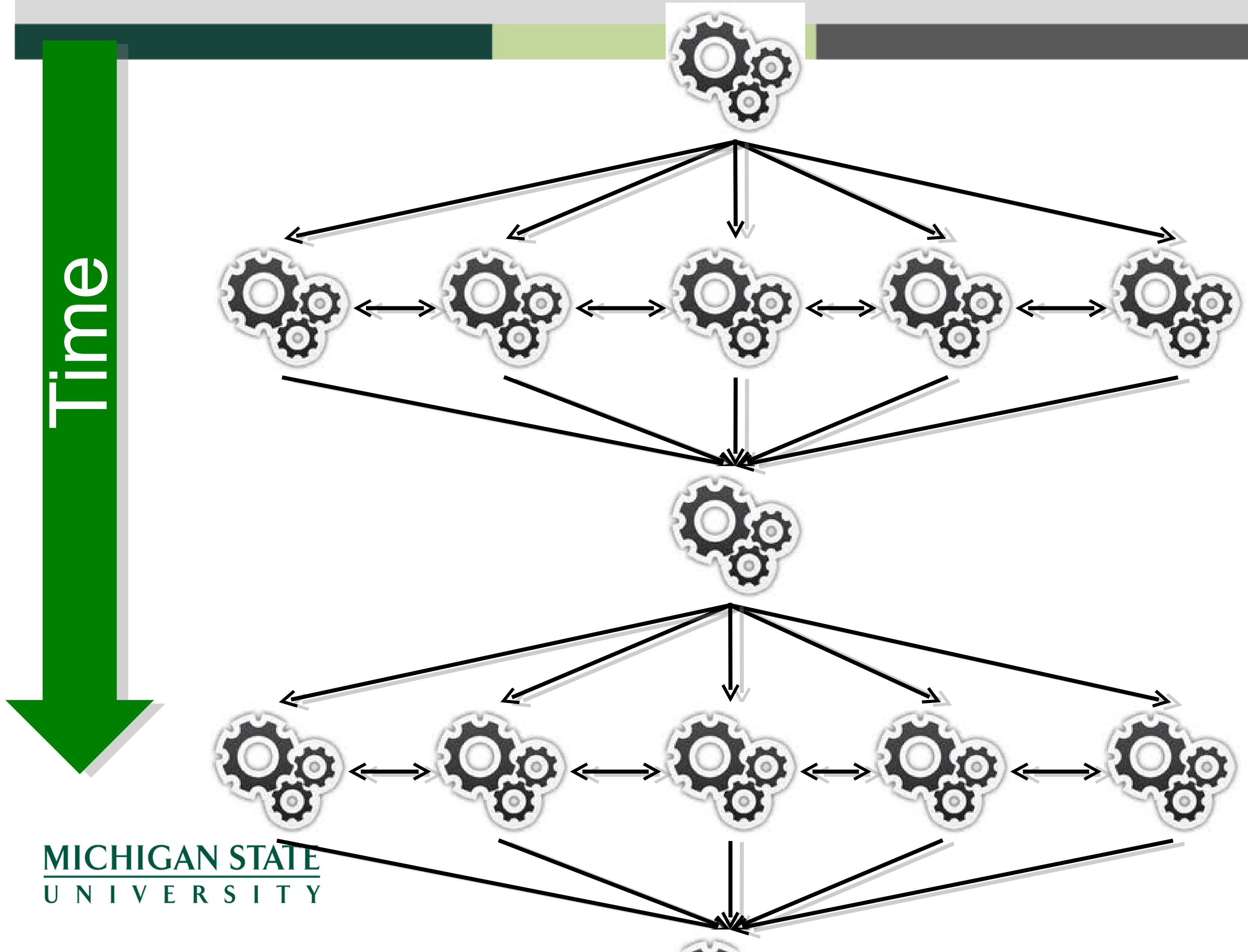
```
#!/bin/bash -login
#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100
cd ${PBS_O_WORKID}
sleep $(( ${RANDOM} % 100 ))

for file in *.in; do
  output=“./${file%.*}.out”
  if [ ! -f ${output} ]; then
    touch ${output}
    ./myprogram ${file} > ${output}
    qsub -t 0 -N ${PBS_JOBNAME} ${0}
    exit 0
  fi
done
```

Loosely Coupled



Tightly Coupled



Shared Memory Parallelization

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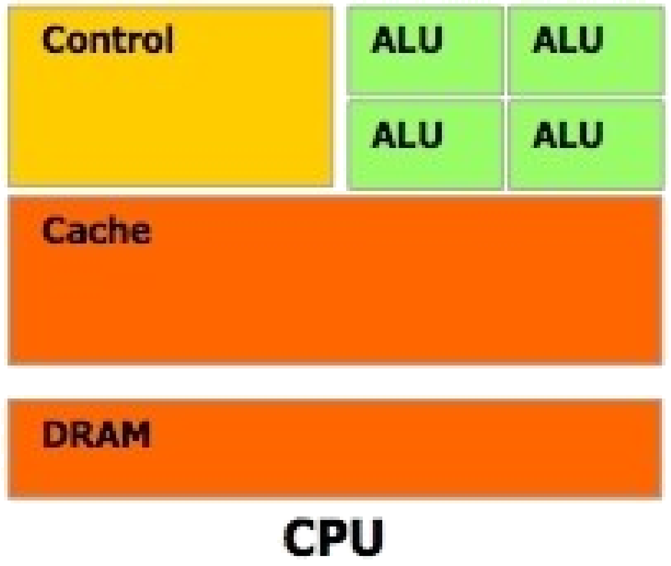
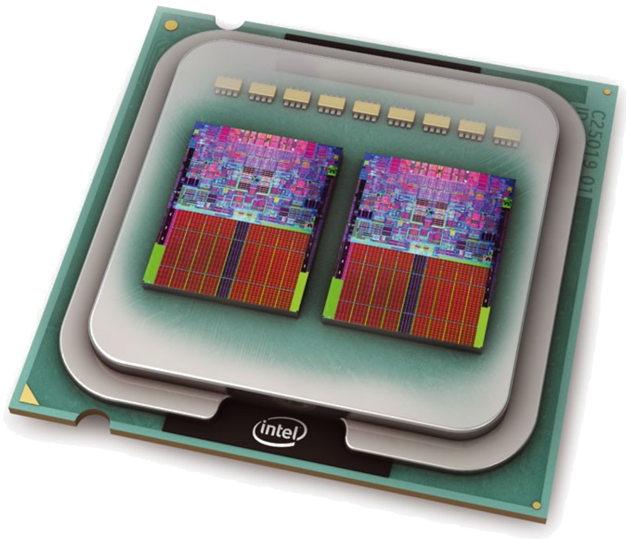
Shared Memory

- Different threads (cores, processes) communicate though pointers to the same memory location
- Problems can occur if different threads write the same memory at the same time
- Flags (also called locks and/or semaphores) are used to allow only one thread to access memory at the same time

Shared Memory Communication

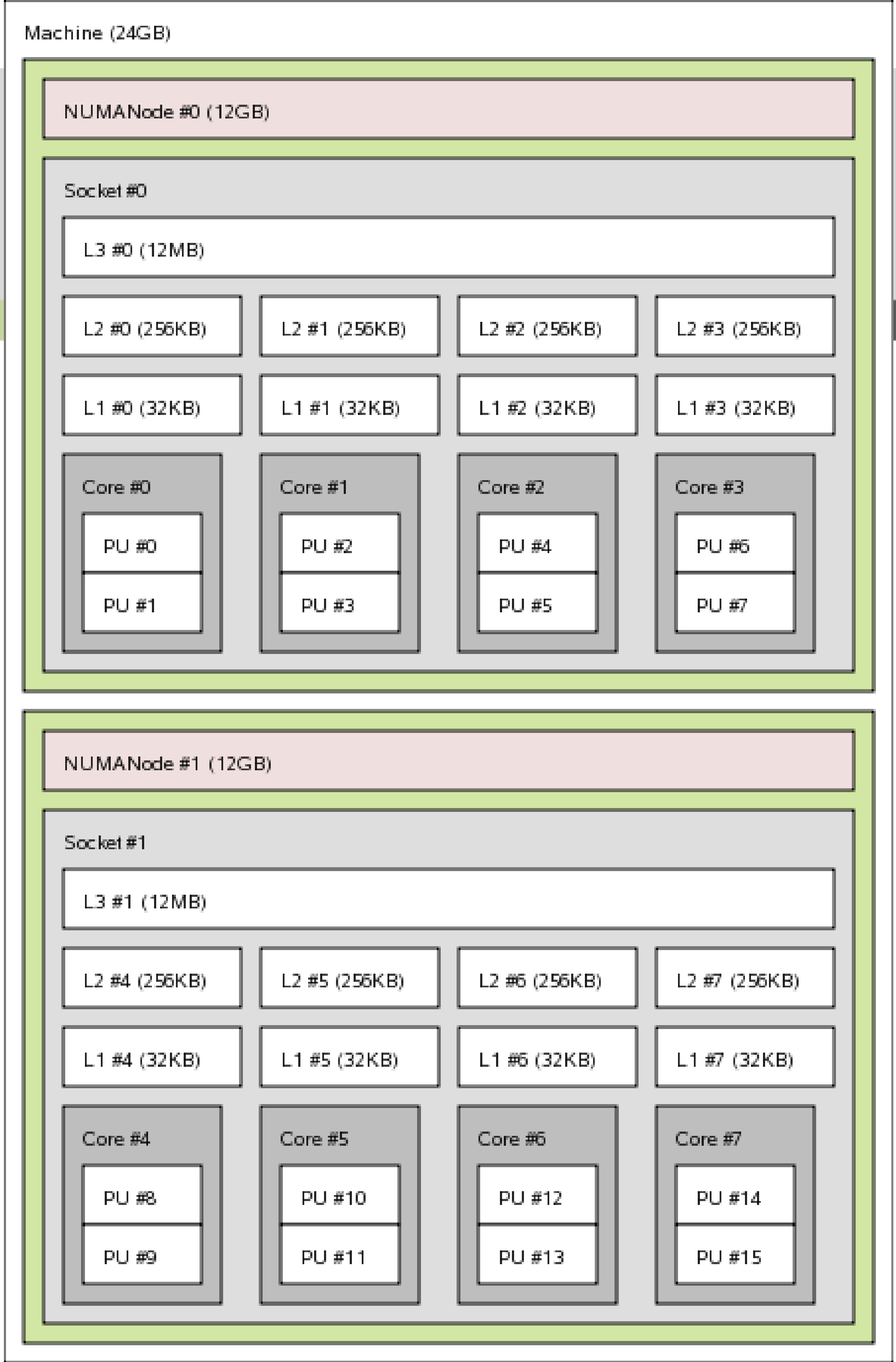
- Cores on a processor share the same memory
- OpenMP
- Fat nodes
  - 96 cores
  - 6TB of memory





Intel10

- 8 cores
- 24 GB memory



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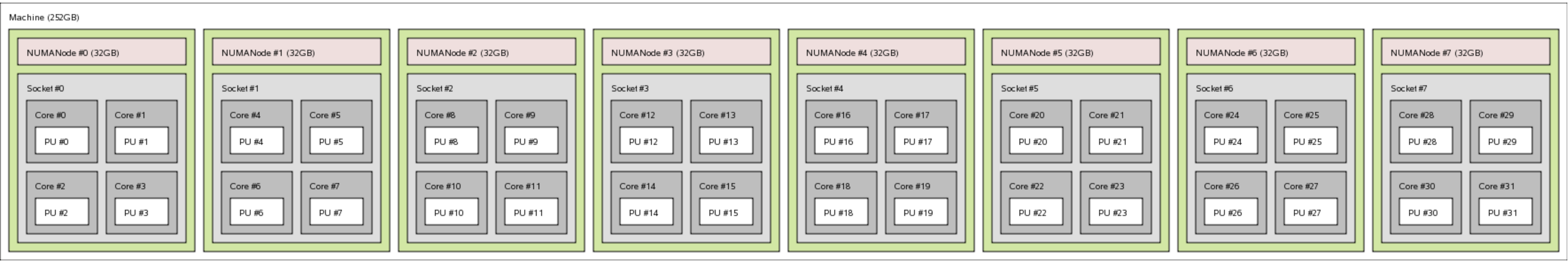
Large Memory Example

- 32 cores
- 256 GB memory



- We also have nodes with up to 64 cores and 2TB of memory

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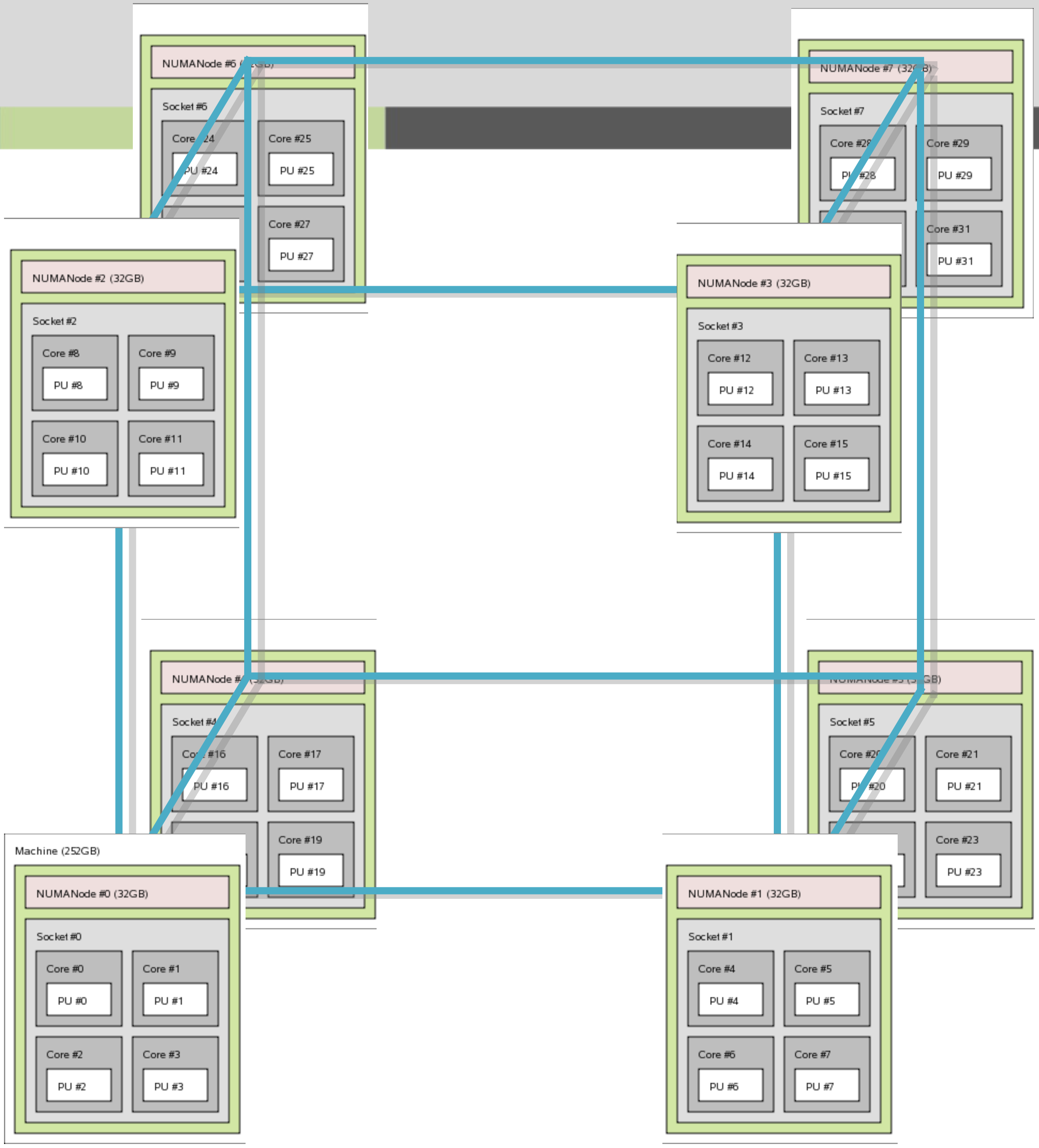
NUMA



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Shared memory submission scripts

- Typically one node with multiple processors per node (ppn)
  - #PBS –l nodes=1:ppn=**8**
- Different programs use different methods to tell them how many processors to use
  - Command line arguments
  - Environment variables

Example: shared memory Script

- Bowtie uses shared memory parallelization
- Get the bowtie example

```
>getexample bowtie
```

- Change to the bowtie directory

```
>cd ./bowtie
```

- Look at the submission script

```
>less ./bowtie.qsub
```

- Run the job

```
>qsub bowtie.qsub
```

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OpenMP

- Common Shared Memory parallelizaiton
- Single program runs in many threads
- Really easy to pick loops that are parallel and split them into multi threads
- Minor modifications to code that can be written not to affect single

OpenMP is easy

```
#include <omp.h>

...
  #pragma omp parallel for
  for (i=0;i<100;++i) {
    A(I) = A(I) + B
  }

...
```

Compile OpenMP Jobs

- Use compiler option fopenmpi.
  - –fopenmp
- Example:

```
gcc –fopenmp mycode.cc –o
  mycode
```

simpleOMP.qsub example

```
#!/bin/bash -login
#PBS -l walltime=00:01:00
#PBS -l nodes=1:ppn=5,feature=gbe

cd ${PBS_O_WORKDIR}
export OMP_NUM_THREADS=${PBS_NUM_PPN}

./simpleOMP

qstat -f ${PBS_JOBID}
```

Try another getexample

```
getexample helloOpenMP
getexample OpenMP_profiling
```

Shared Network Parallelization

MPI on HPCC

- Two Flavors of MPI
- Switching flavors and compiling
- Running in a script
- Running on the developer nodes

MPI program (1 of 4)

```
/* Needed for printf'ing */
#include <stdio.h>
#include <stdlib.h>

/* Get the MPI header file */
#include <mpi.h>

/* Max number of nodes to test */
#define max_nodes 264

/* Largest hostname string hostnames */
#define str_length 50
```

MPI program (2 of 4)

```
int main(int argc, char **argv)
{
   /* Declare variables */
   int   proc, rank, size, namelen;
   int   ids[max_nodes];
   char  hostname[str_length][max_nodes];
   char  p_name[str_length];

   MPI_Status status;
   MPI_Init(&argc, &argv);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
   MPI_Comm_size(MPI_COMM_WORLD, &size);
   MPI_Get_processor_name(p_name,&namelen);
```

MPI program (3 of 4)

```
if (rank==0) {
   printf("Hello From: %s I am the receiving processor
%d of %d\n",p_name, rank+1, size);
   for (proc=1;proc<size;proc++) {
      MPI_Recv(&hostname[0][proc], \\
               str_length,MPI_INT,proc, \\
               1,MPI_COMM_WORLD,&status);
      MPI_Recv(&ids[proc], \\
               str_length,MPI_INT,proc, \\
               2,MPI_COMM_WORLD,&status);
      printf("Hello From: %-20s I am processor %d of
%d\n",&hostname[0][proc], ids[proc]+1, size);
   }
```

MPI program (4 of 4)

```
} else { // NOT Rank 0
      srand(rank);
      int t = rand()%10+1;
      sleep(t);
      MPI_Send(&p_name,str_length, \\
               MPI_INT,0,1,MPI_COMM_WORLD);
      MPI_Send(&rank,str_length, \\
               MPI_INT,0,2,MPI_COMM_WORLD);
   }
   MPI_Finalize();

   return(0);
}
```

Two Flavors of MPI

- **mvapich** vs **openmpi** (default)
- Historically **mvapich** was much faster that **openmpi**
- The newest version of **openmpi** is just as fast as **mvapich**
- I feel that **openmpi** is much easier to use, but either will work on HPCC

Switching Flavors

- Use the "module" command to switch between the two versions of mpi
- **Openmpi** module is loaded by default
- To switch to mvapich you first need to unload **openmpi**:

```
> module unload OpenMPI
```

- Then you need to load **mvapich:**

```
> module load MVAPICH
```

- You can do both commands in one step by using swap:

```
> module swap OpenMPI MVAPICH
```

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MPI Submission Scripts

openmpi

```
#!/bin/bash -login
#PBS -l nodes=10:ppn=1
cd ${PBS_O_WORKDIR}
mpirun <program_name>
```

mvapich

```
#!/bin/bash -login
#PBS -l nodes=10:ppn=1
cd ${PBS_O_WORKDIR}
module swap OpenMPI MVAPICH
mpiexec <program_name>
```

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Trying out an example

1. Log on to one of the developer nodes
2. Load the powertools module:

```
>   module load powertools
```

1. Run the getexample program. This will create a folder called helloMPI:

```
>   getexample helloMPI
```

1. Change to the helloMPI directory and read the readme files
2. Or just type the following on the command line:

```
>   ./README
```

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Testing MPI jobs on dev node

- Use mpirun instead of mpiexec
- Need a hostfile

```
> echo $HOST >> ./hostfile
> echo $HOST >> ./hostfile
> echo $HOST >> ./hostfile
> echo $HOST >> ./hostfile
```

- MPIRUN example:

```
> mpirun –np 4 –hostfile ./hostfile helloMPI
```

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Running on the Command Line

- The scheduler automatically knows how many and where to run MPI processes.
- However, on the command line, you need to specify the nodes and processors.
- **openmpi** and **mvapich** are a little different.

Command Line Differences

- Openmpi
  - **mpirun**
  - Default assumes one process on the current host.
  - You do not even need the **mpirun** command to run the default.
  - Optionally you can use the –n and –hostfile options to change the default

- mvapich
  - **mpirun**
  - Requires both the –np and –machinefile flag to run.

Command line

- mvapich

```
mpirun -np 4 -machinefile machinefile <program_name>
```

- openmpi

```
mpirun -n 4 -hostfile machinefile <program_name>
```

- NOTE: I did a check and either MPI implementation will work with either notation.

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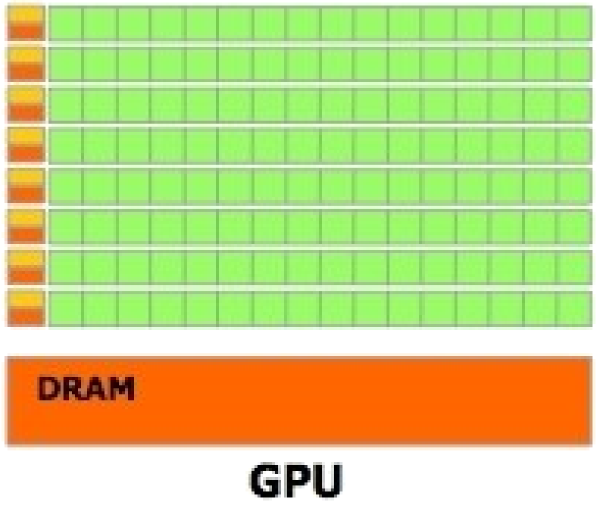
Which MPI command do you use?

	Command Line	Job Script
openmpi	mpirun	mpirun
mvapich	mpirun	mpiexec

Accelerator Cards

GPU

- Cards used to render graphics on a computer
- Hundreds of cores
- Not very smart cores
- But, if you can make your research look like graphics rendering you may be able to run really fast!



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Running on the GPU

- Program Starts on the CPU
  - Copy data to GPU (slow-ish)
  - Run kernel threads on GPU (very fast)
  - Copy results back to CPU (slow-ish)

- There are a lot of clever ways to fully utilize both the GPU and CPU.

Pros and Cons

- Benefits
  - Lots of processing cores.
  - Works with the CPU as a co-processor
  - Very fast local memory bandwidth
  - Large online community of developers

- Drawbacks
  - Can be difficult to program.
  - Memory Transfers between GPU and CPU are costly (time).
  - Cores typically run the same code.
  - Errors are not detected (on older cards)
  - Double precision calculations are slow (On older cards)

CUDA program (1 of 5)

```
#include "cuda.h"
#include <iostream>

using namespace std;

void printGrid(float an_array[16][16]) {
  for (int i = 0; i < 16; i++){
      for (int j = 0; j < 16; j++) {
          cout << an_array[i][j];
      }
      cout << endl;
    }
}
```

CUDA program (2 of 5)

```
__global__ void theKernel(float * our_array)
{
  // This is array flattening,
  //(Array Width * Y Index + X Index)
  our_array[(gridDim.x * blockDim.x) * \\
            (blockIdx.y * blockDim.y + threadIdx.y) + \\

            (blockIdx.x * blockDim.x + threadIdx.x)] = \\
           = 5;
}
```

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CUDA program (3 of 5)

```
int main()
{
  float our_array[16][16];

  for (int i = 0; i < 16; i++) {
    for (int j = 0; j < 16; j++) {
      our_array[i][j] = 0;
    }
  }
```

CUDA program (4 of 5)

```
//STEP 1: ALLOCATE
float * our_array_d;
int size = sizeof(float)*256;
cudaMalloc((void **) &our_array_d, size);

//STEP 2: TRANSFER
cudaMemcpy(our_array_d, our_array, size, \\
                    cudaMemcpyHostToDevice);
```

CUDA program (5 of 5)

```
   //STEP 3: SET UP
   dim3 blockSize(8,8,1);
   dim3 gridSize(2,2,1);

   //STEP 4: RUN
   theKernel<<<gridSize, blockSize>>>(our_array_d);

   //STEP 5: TRANSFER
   printGrid(our_array);
   cudaMemcpy(our_array, our_array_d, size, \\
              cudaMemcpyDeviceToHost);
   cout << "--------------------" << endl;
   printGrid(our_array);


}
```

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Compile CUDA Jobs

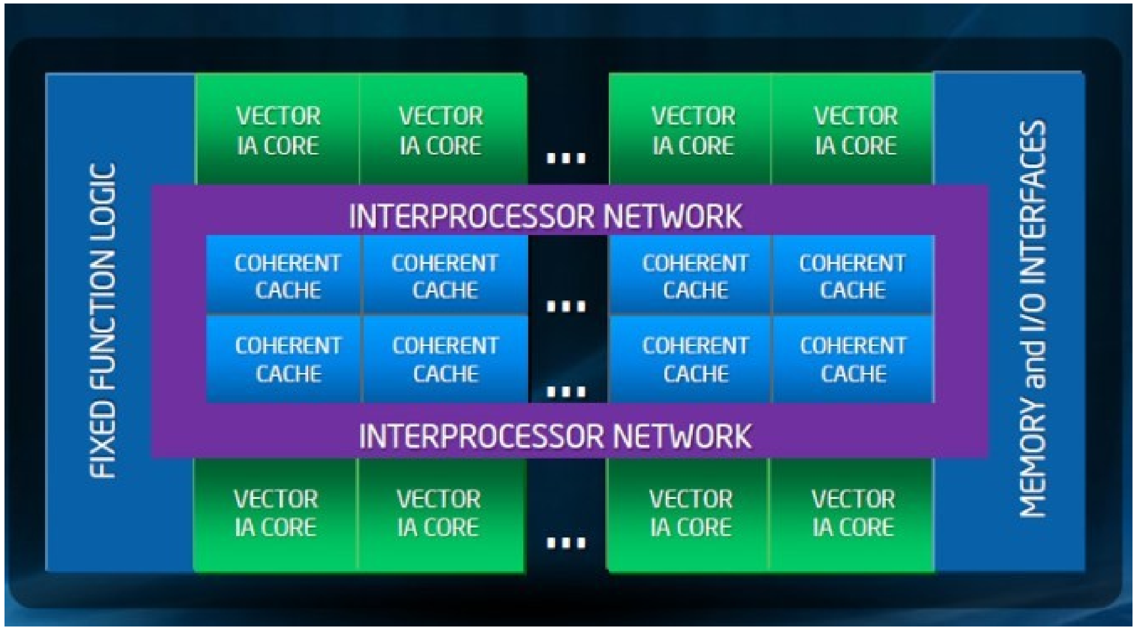
- Just like MPI, to compile an cuda program you need to use the cuda compiler wrappers:
  - nvcc simple.cu -o simple_cuda

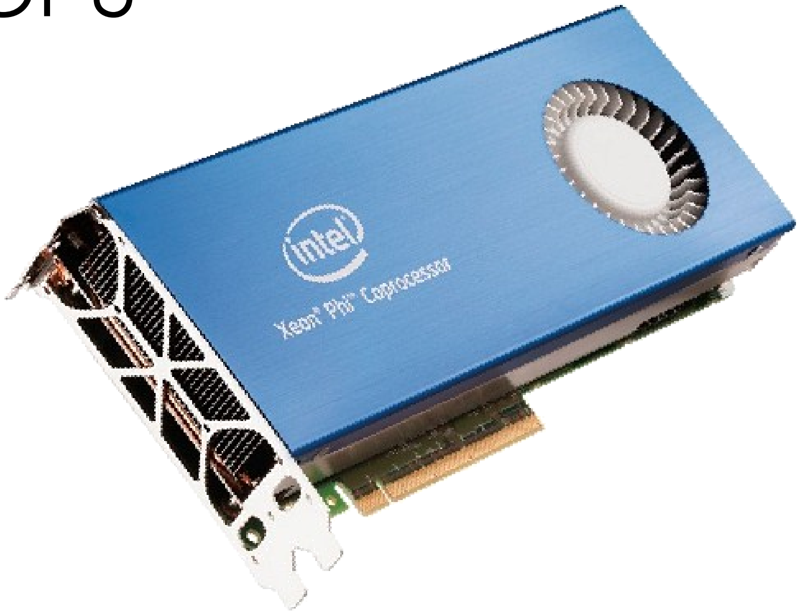
Try a cuda getexample

```
getexample cuda
getexample cuda_clock
getexample cuda_hybrid
getexample NAMD_CUDA_example
```

Intel Xeon Phi

- Cross between CPU and GPU
- About 61 Pentium III cores
  - Less cores/slower than GPU
  - Easier to use than GP





- MPI
- OPenMP

Try a Phi Card example

```
getexample MIC_examples
getexample MKL_mic
```

Standard Libraries

Standard Libraries

- When possible take advantage of parallel libraries
  - Easy to use
  - Saves time
  - Takes care of the parallel coding for you
  - Tested and vetted by the community

Math Kernel Library

- getexample MKL_benchmark
- getexample MKL_c_eigenvalues
- getexample MKL_Example
- getexample MKL_mic
- getexample MKL_parallel

Other Libraries

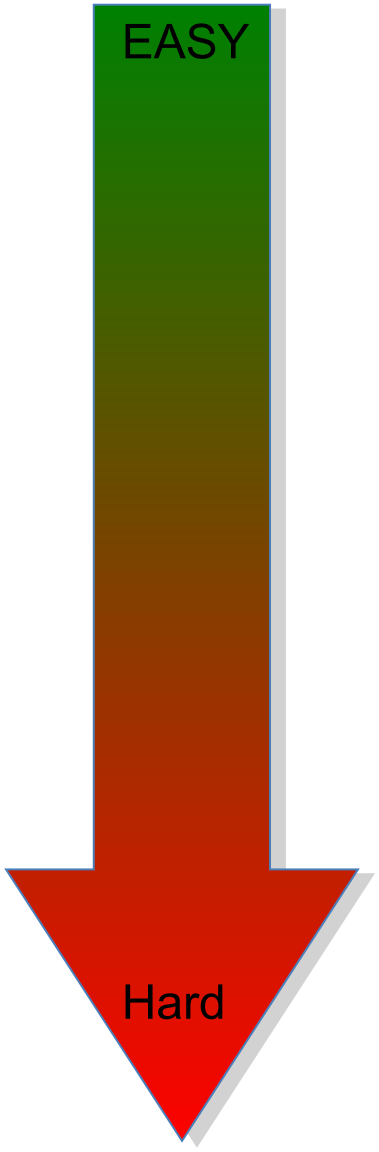
- Fftw
- BLAS
- ACML
- BLAS (Basic Linar Algibra
- Lapak
- trilinos
- petci
- Magma

Which approach is the best?

- Depends on what you are doing?
- Depends on how much communication you need.
- Depends on what hardware you have.
- Depends on how much time you have.

My Recommendations

- Pleasantly Parallel
- Standard Libraries
- OpenMP
- OpenACC
- OpenMP on Phi
- MPI
- MPI on Phi?
- GPGPU



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Agenda

- Overview
- Advanced System Description
- Powertools
- Doing more faster
  - Pleasantly Parallel, Shared Memory, Shared Network, Accelerators, Standard Libraries
- **Tricks and tips**

Tips and Tricks
Going beyond system Limits

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- Going beyond system Limits
  - More than 520 jobs
  - Jobs longer than 1 week
  - Taking advantage of more nodes

Finding more Nodes

- Owners are guaranteed access to their buy-in node within 4 hours. If they are not using the node, others can use it:
  - #PBS –l walltime=04:00:00
- Some of the nodes do not have Infiniband. If you are not using scratch and do not need between node communication you can access these nodes:
  - #PBS feature=gbe

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Checkpoint / Restart

- What?
  - Save the state of your program
  - Restart your program from the saved point
- How?
  - Design into your program
  - BLCR (Berkley Lab Checkpoint Restart)
  - Condor Checkpoint Restart
  - Others
- Why?
  - Robust jobs
    - As HPC scales … hardware failures are guaranteed
  - Longer jobs
  - Better science

Getting Help

- Documentation and User Manual – wiki.hpcc.msu.edu
- Contact HPCC and iCER Staff for:
  - Reporting System Problems
  - HPC Program writing/debugging Consultation
  - Help with HPC grant writing
  - System Requests
  - Other General Questions
- Primary form of contact - http://contact.icer.msu.edu/
- HPCC Request tracking system – rt.hpcc.msu.edu
- HPCC Phone – (517) 353-9309
- HPCC Office – 1400 PBS
- Open Office Hours – 1pm Monday (BPS 1440)

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